Overview of Fuel Cell Projects in the Materials and Process Simulation Center


Materials and Process Simulation Center, California Institute of Technology
1200 E. Colorado Blvd., m/c 139-74, Pasadena, CA 91125, USA

Fuel cell research in the Materials and Process Simulation Center covers a broad area from low-temperature Polymer Electrolyte Membrane Fuel Cells (PEMFCs) based on hydrated Nafion up to high-temperature Solid Oxide Fuel Cells (SOFCs) with Y-stabilized zirconia oxide-ion conductor and Y-doped BaZrO$_3$ proton conductor as electrolytes, and includes electrode catalysts such as Pt, Pt-alloys, and Ni. Alternative membranes based on imidazole, dendrimers, solid acids, and zeolites, as well as prospective materials for hydrogen storage, are also of our interest.

The goal of our computational work is to develop an atomistic model of a fuel cell system based on the application of first-principles theory and useful for prototyping new systems computationally prior to experiment. First principles mean that we must start with quantum mechanics (QM). However, computational modeling of fuel cell processes at realistic operating conditions requires systems with thousands of atoms. We propose to address such problems using recently developed first-principles based rational approaches that enable to describe chemical processes at suitable scales. The critical component of our approach is the overlapping simulation methodologies, in which QM data are used to train the first-principles based ReaxFF reactive force field. The ReaxFF has ability to describe formation and dissociation of chemical bonds, which can be used for large-scale molecular dynamics (MD) simulations to characterize properties of the fuel cell systems. Recently, the ReaxFF has been re-coded for a parallel environment and completely reactive simulations of about half a billion atoms have been reported [1], which allow realistic simulations of the complex fuel cell chemistry to be carried out.

For the most rapid progress, it is essential to couple these computational efforts to experimental tests of the predictions with the results of subsequent experiments fed back into the theory, perhaps leading to refined simulations aimed at resolving discrepancies or considering new phenomena. Ultimately this process of developing a complete computational model whose predictions have been validated by experiment will allow an accurate fuel cell model to be developed based on the theory and simulations but incorporating all the results obtained from experiments.

References